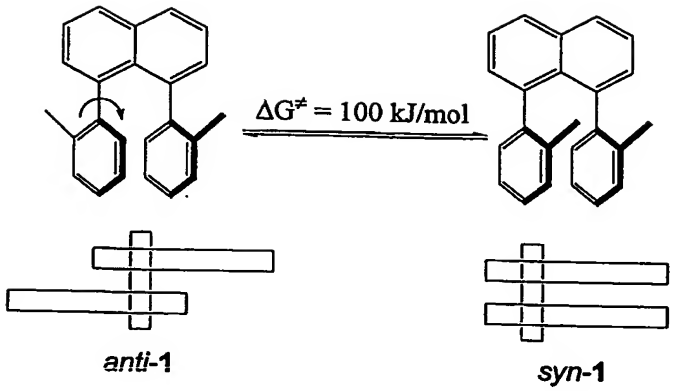
Figure 1



BEST AVAILABLE COPY

Figure 2

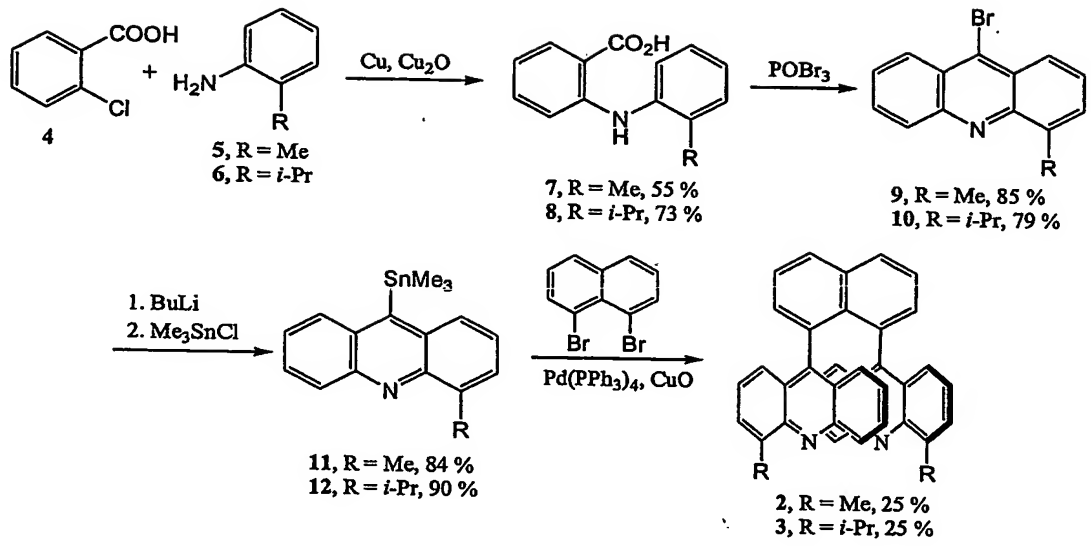

COOH
Cl
4
H_2N
R
5, R = Me
6, R = i-Pr
Cu, Cu_2O
CO_2H
N
H
R
7, R = Me, 55 %
8, R = i-Pr, 73 %
$POBr_3$
Br
N
R
9, R = Me, 85 %
10, R = i-Pr, 79 %
1. BuLi
2. Me_3SnCl
$SnMe_3$
N
R
11, R = Me, 84 %
12, R = i-Pr, 90 %
Br Br
$Pd(PPh_3)_4$, CuO
N
N
R
R
2, R = Me, 25 %
3, R = i-Pr, 25 %

Figure 3

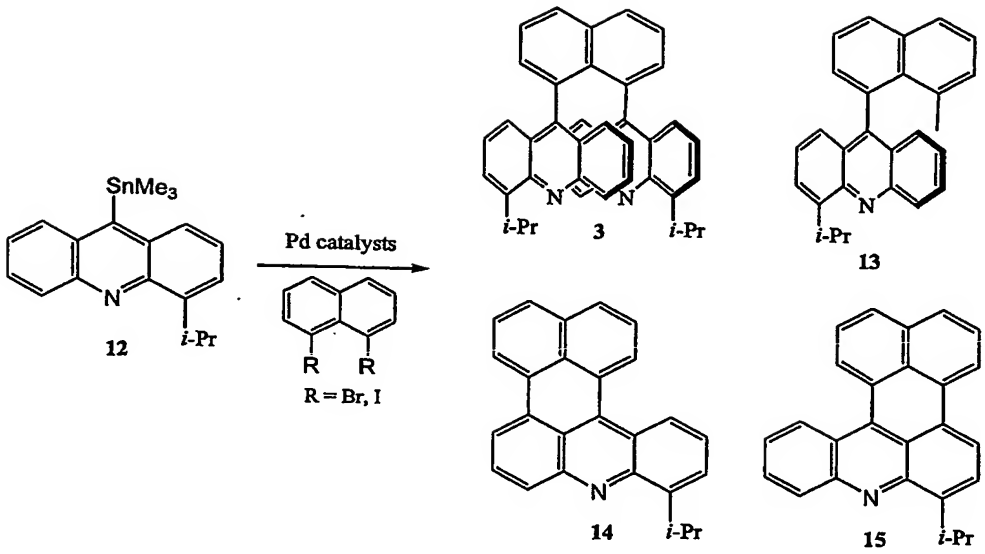

SnMe3
N
i-Pr
12
Pd catalysts
R R
R = Br, I
N
N
i-Pr
3
i-Pr
N
i-Pr
13
N
14
i-Pr
N
15
i-Pr

Figure 4

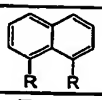
entry		stannane	Catalyst (mol%)	additives	yield of major product (%)
1	R = I	**12**	$Pd(PPh_3)_4$ (10)[a]	/	**14** + **15** (17)
2	R = I	**12**	$Pd(PPh_3)_4$ (10)[a]	Cy_2NMe	**14** + **15** (17)
3	R = Br	**12**	$Pd(PPh_3)_4$ (10)[b]	CuO	**3** (5)
4	R = Br	**12**	$Pd(PPh_3)_4$ (10)[c]	CuO	**3** (5)
5	R = Br	**12**	$Pd(PPh_3)_4$ (10)[a]	CuO	**3** (10)
6	R = Br	**12**	$Pd(PPh_3)_4$ (20)[a]	CuO	**3** (18)
7	R = Br	**12**	$Pd(PPh_3)_4$ (30)[a]	CuO	**3** (25)
8	R = Br	**12**	$Pd(PPh_3)_4$ (40)[a]	CuO	**3** (25)
9	R = Br	**12**	$Pd(PPh_3)_4$ (50)[a]	CuO	**3** (25)
10	R = Br	**11**	$Pd(PPh_3)_4$ (30)[a]	CuO	**2** (25)

Figure 5

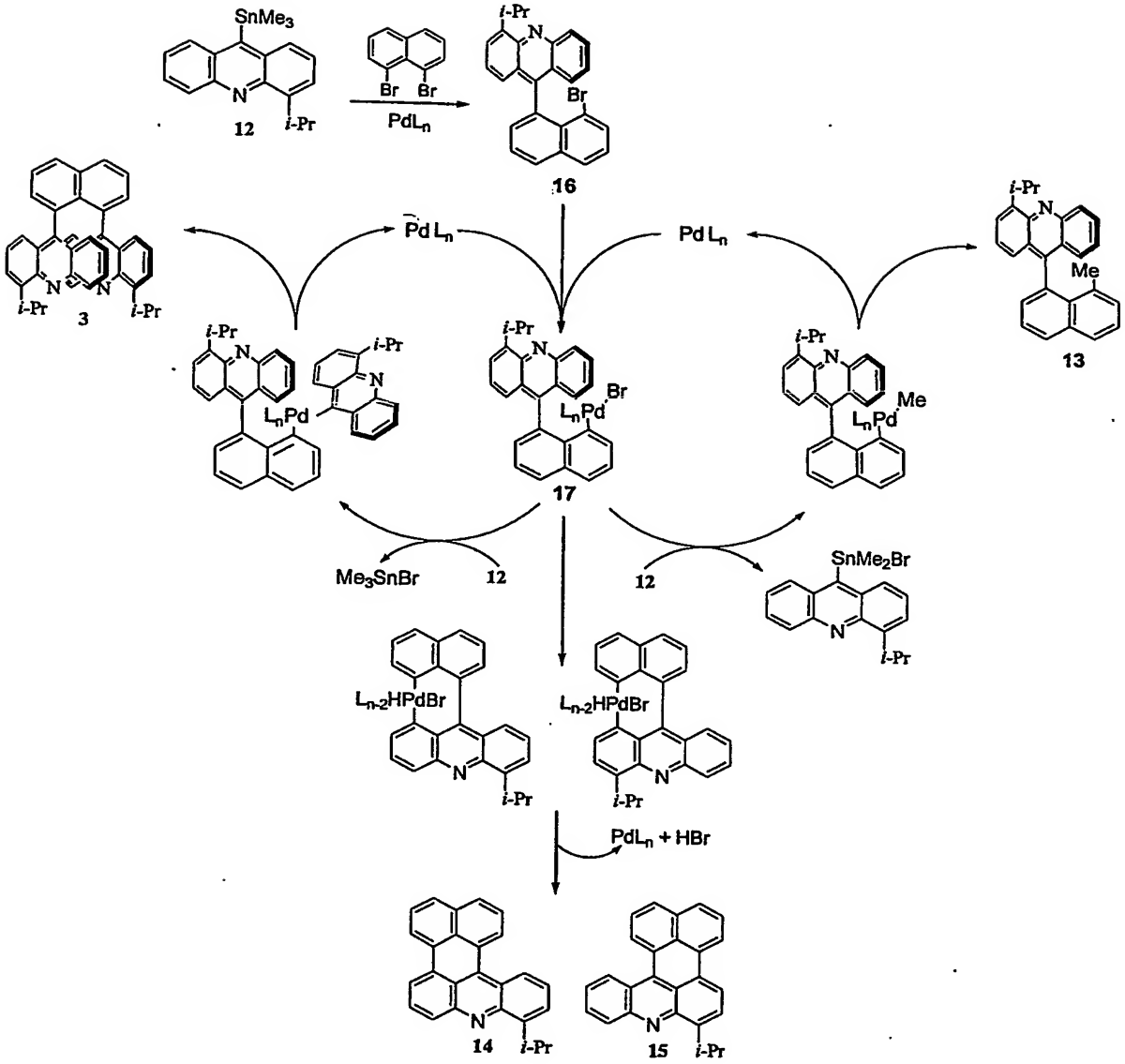

SnMe3
12
i-Pr
Br Br
PdLn
16
Br
PdLn
PdLn
3
i-Pr
N
LnPd
LnPd
Br
17
LnPd
Me
13
Me
Me3SnBr
12
12
SnMe2Br
Ln-2HPdBr
Ln-2HPdBr
PdLn + HBr
14
15

Figure 6

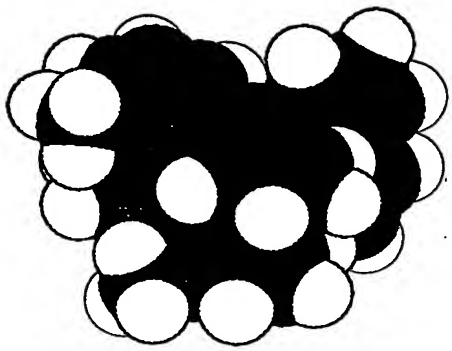


Figure 7

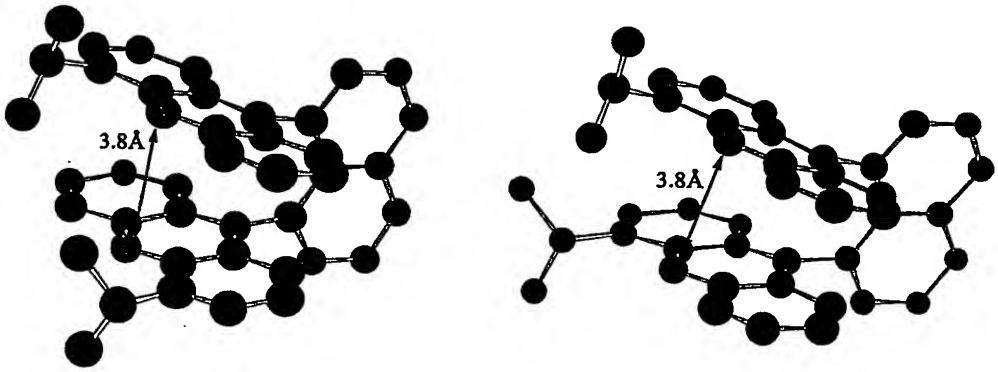


Figure 8

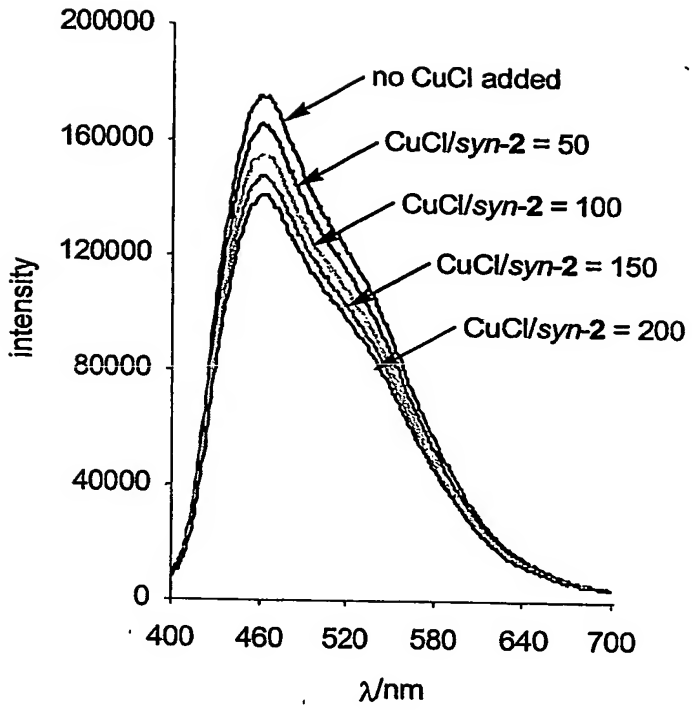

200000
160000
120000
80000
40000
0
intensity
400
460
520
580
640
700
λ/nm
no CuCl added
CuCl/*syn*-**2** = 50
CuCl/*syn*-**2** = 100
CuCl/*syn*-**2** = 150
CuCl/*syn*-**2** = 200

Figure 9

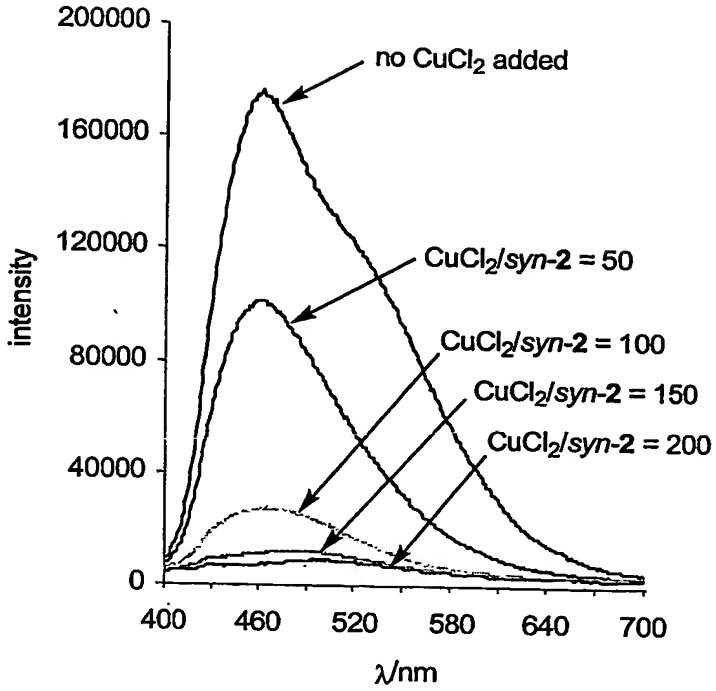

200000
160000
120000
80000
40000
0
intensity
400
460
520
580
640
700
λ/nm
no CuCl2 added
CuCl2/syn-2 = 50
CuCl2/syn-2 = 100
CuCl2/syn-2 = 150
CuCl2/syn-2 = 200

Figure 10

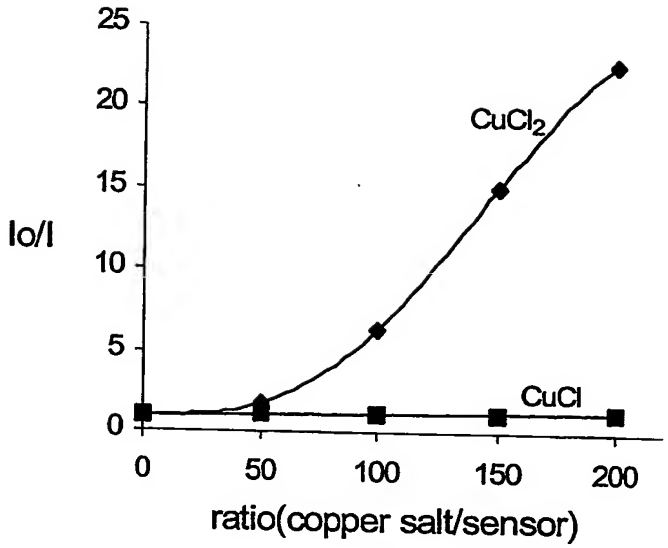

25
20
15
10
5
0
Io/I
CuCl2
CuCl
0
50
100
150
200
ratio(copper salt/sensor)

Figure 11

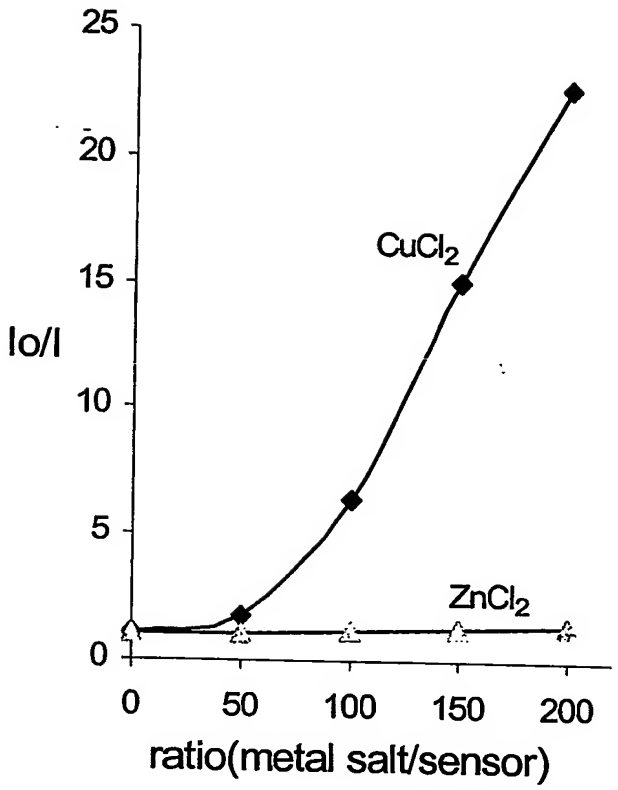

25
20
15
10
5
0
Io/I
CuCl2
ZnCl2
0
50
100
150
200
ratio(metal salt/sensor)

Figure 12

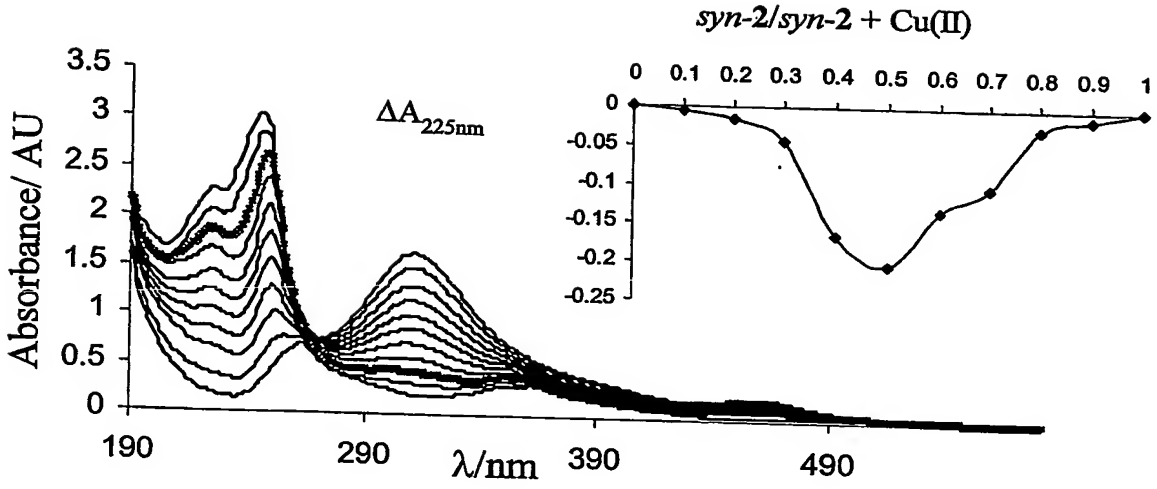

syn-2/syn-2 + Cu(II)
ΔA225nm
Absorbance/ AU
λ/nm
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
-0.05
-0.1
-0.15
-0.2
-0.25

Figure 13

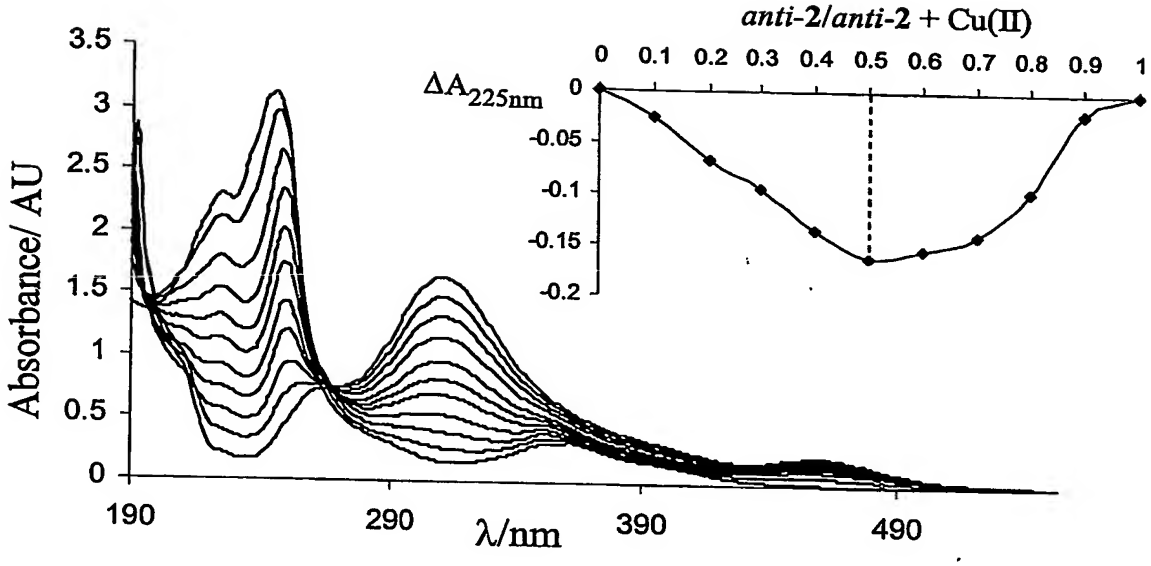

anti-2/anti-2 + Cu(II)
ΔA225nm
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
-0.05
-0.1
-0.15
-0.2
Absorbance/ AU
3.5
3
2.5
2
1.5
1
0.5
0
190
290
390
490
λ/nm

Figure 14

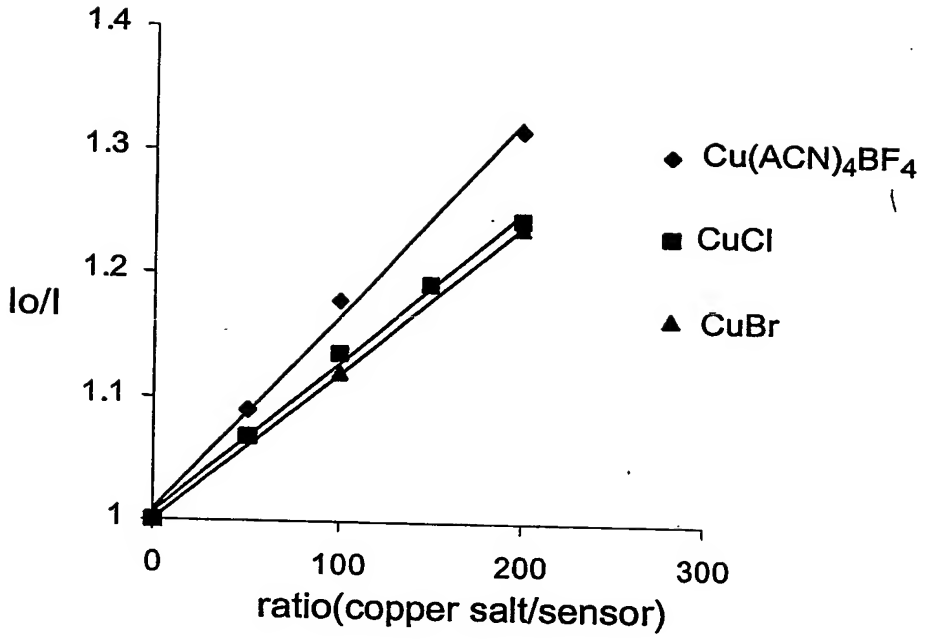

1.4
1.3
1.2
1.1
1
Io/I
0
100
200
300
ratio(copper salt/sensor)
Cu(ACN)4BF4
CuCl
CuBr

Figure 15

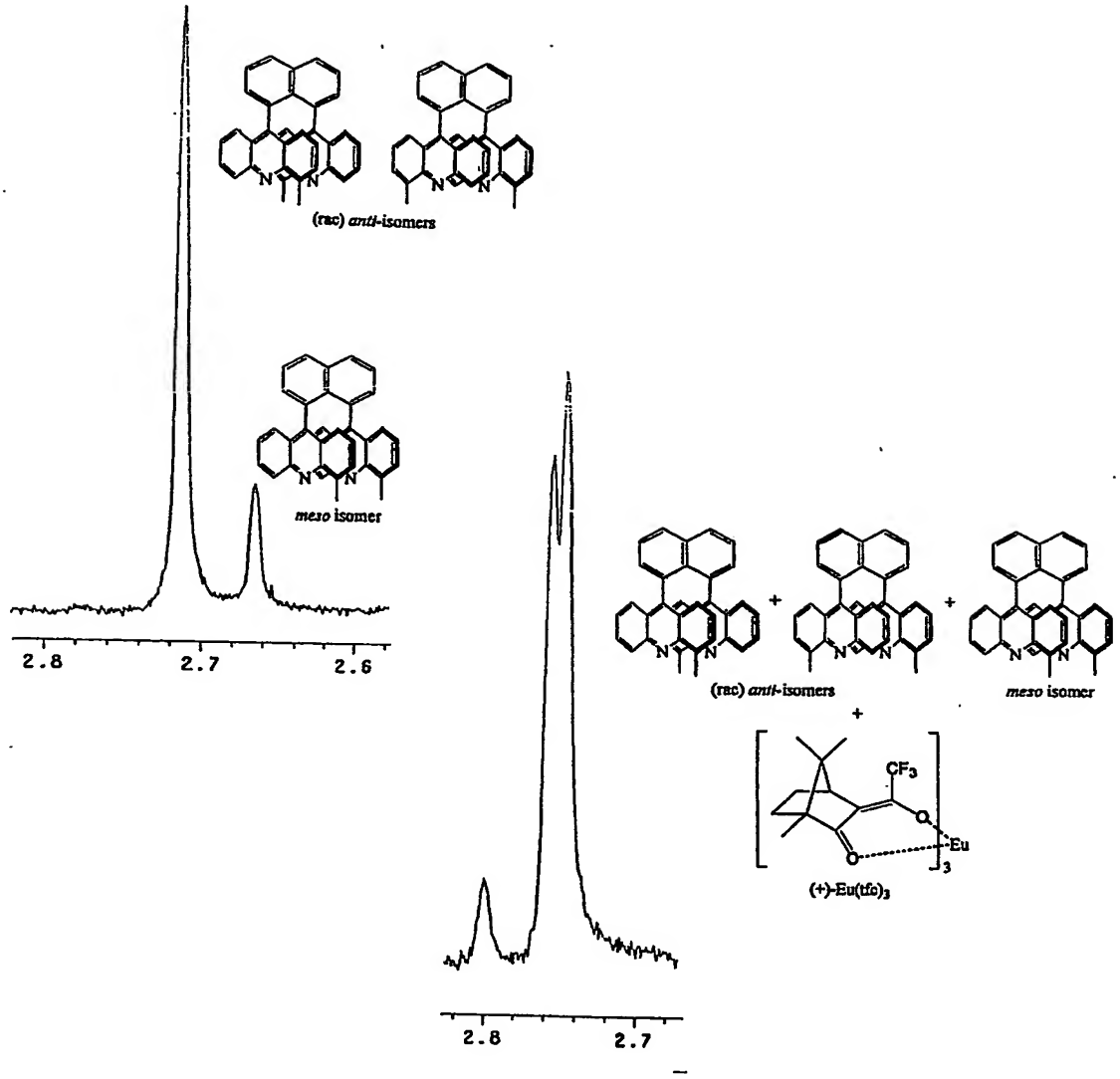

(rac) anti-isomers
meso isomer
2.8
2.7
2.6
(rac) anti-isomers
meso isomer
CF3
O
Eu
3
(+)-Eu(tfc)3
2.8
2.7

Figure 16

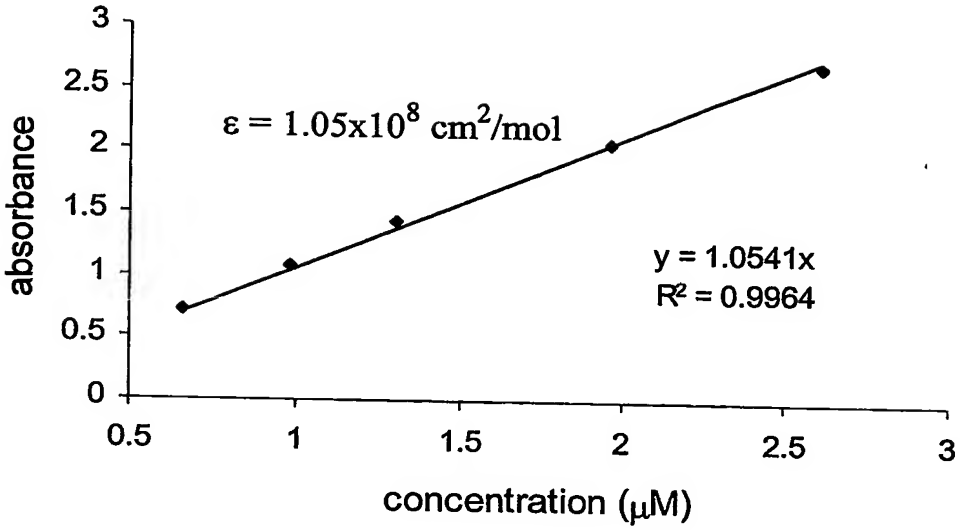

absorbance
concentration (μM)
ε = 1.05x10^8 cm^2/mol
y = 1.0541x
R² = 0.9964
0
0.5
1
1.5
2
2.5
3
0.5
1
1.5
2
2.5
3

Figure 17

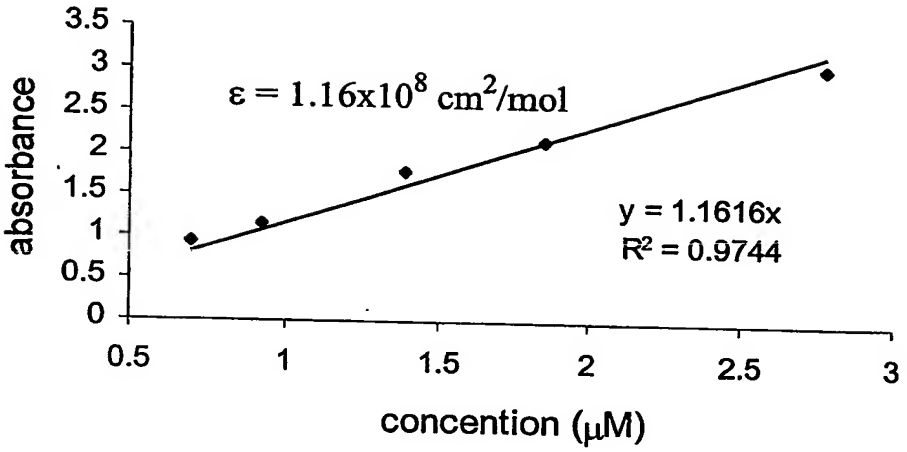

absorbance
3.5
3
2.5
2
1.5
1
0.5
0
0.5
1
1.5
2
2.5
3
concention (μM)
ε = 1.16x10^8 cm^2/mol
y = 1.1616x
R^2 = 0.9744

Figure 18

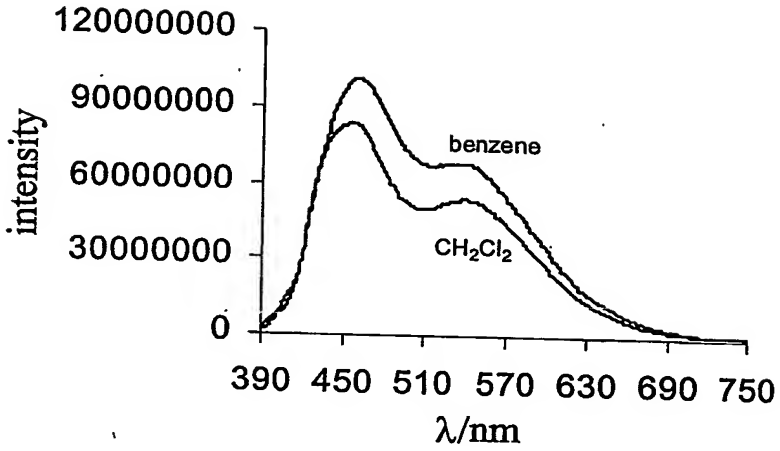

120000000
90000000
60000000
30000000
0
intensity
benzene
CH_2Cl_2
390 450 510 570 630 690 750
λ/nm

Figure 19

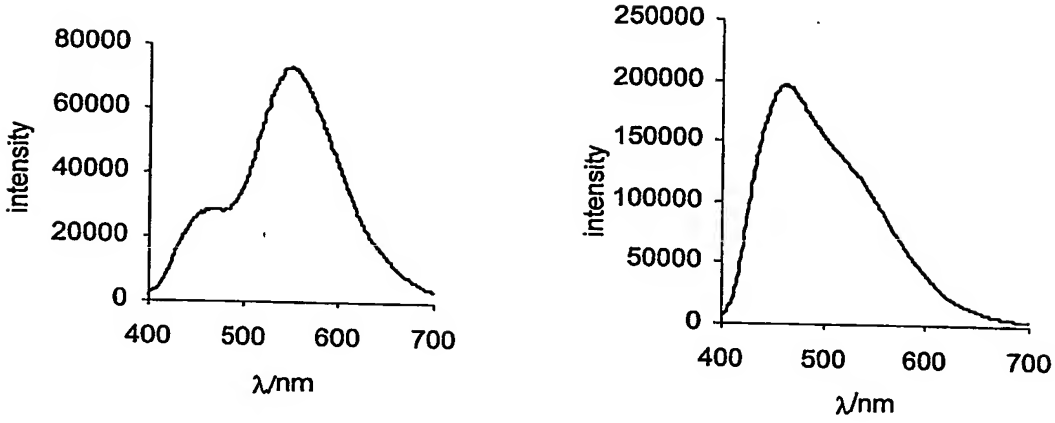

80000
60000
40000
20000
0
intensity
400
500
600
700
λ/nm
250000
200000
150000
100000
50000
0
intensity
400
500
600
700
λ/nm

Figure 20

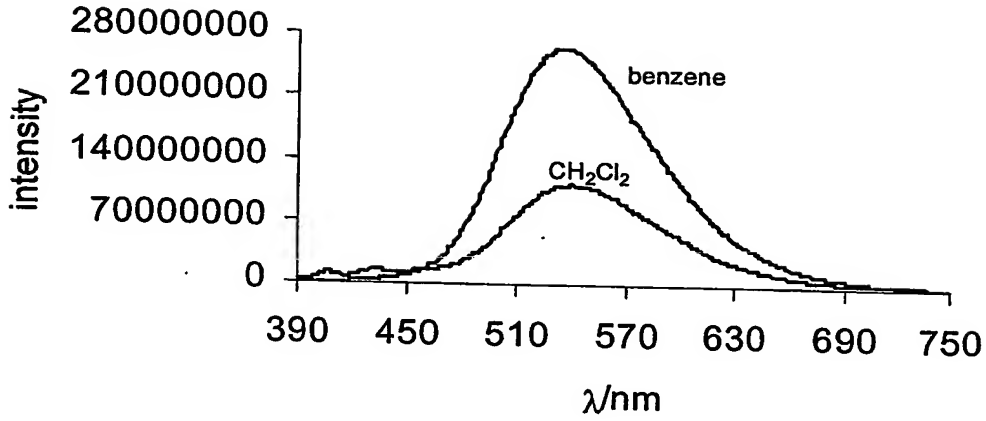
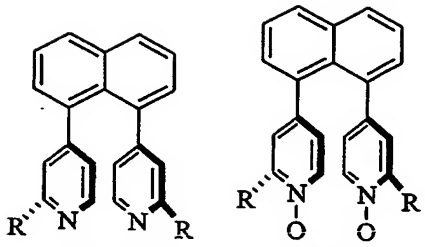

280000000
210000000
140000000
70000000
0
intensity
benzene
CH_2Cl_2
390
450
510
570
630
690
750
λ/nm

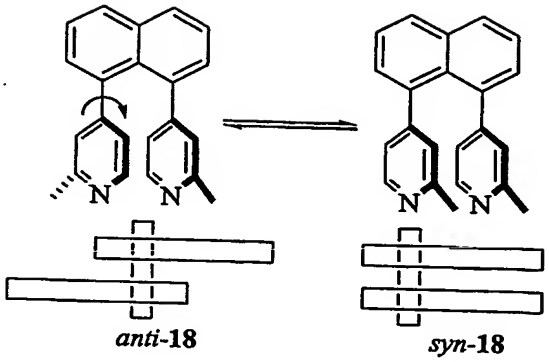
Figure 21



18: R=Me
19: R=Ph

20: R=Me
21: R=Ph

Figure 22



anti-**18** *syn*-**18**

Figure 23

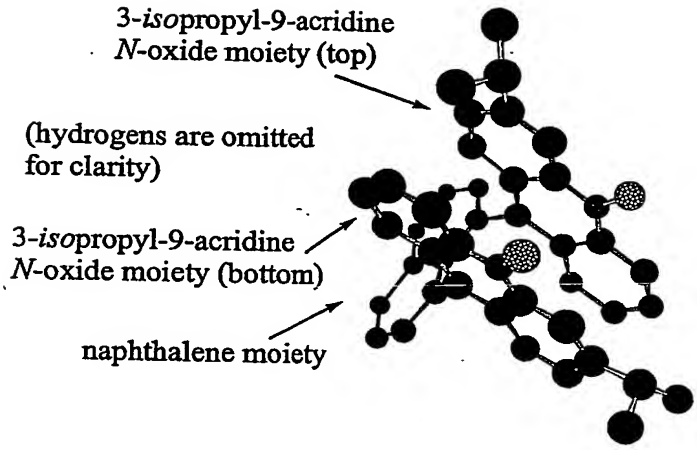

3-*iso*propyl-9-acridine
N-oxide moiety (top)
(hydrogens are omitted
for clarity)
3-*iso*propyl-9-acridine
N-oxide moiety (bottom)
naphthalene moiety

Figure 24

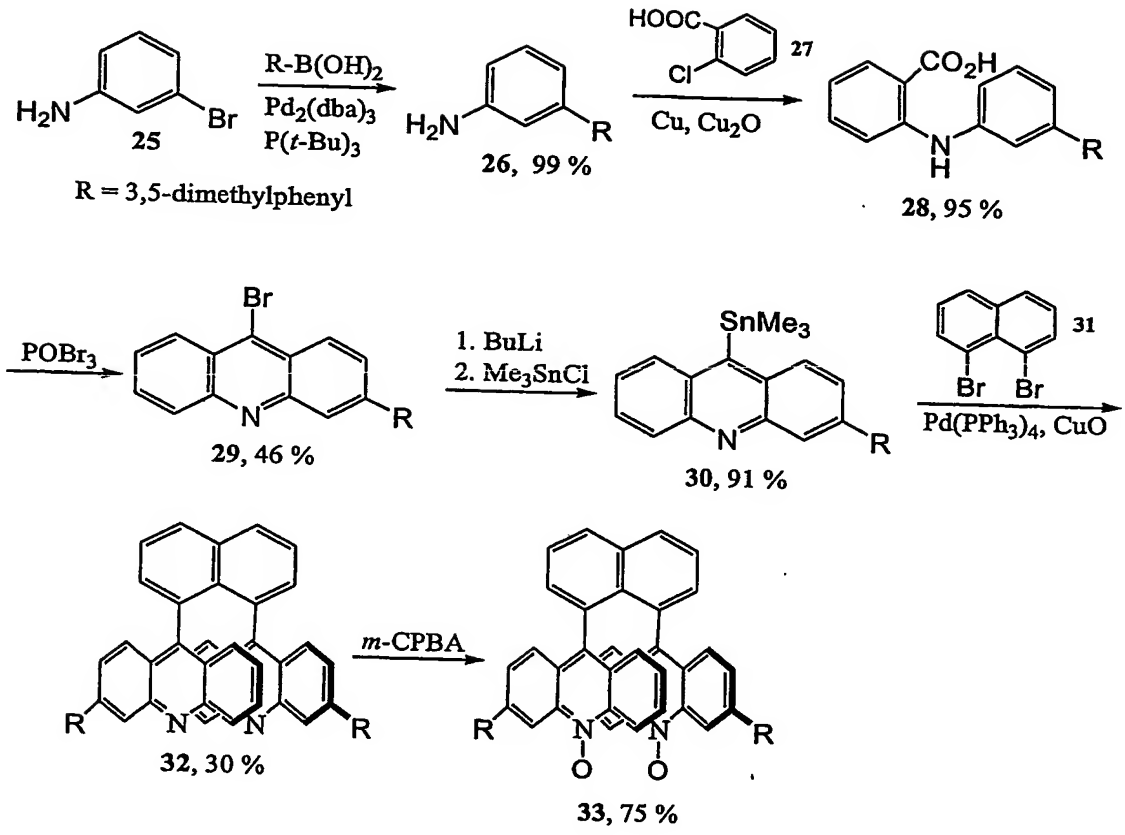

H2N
Br
25
R-B(OH)2
Pd2(dba)3
P(t-Bu)3
H2N
R
26, 99 %
HOOC
Cl
27
Cu, Cu2O
CO2H
N
H
R
28, 95 %
POBr3
Br
N
R
29, 46 %
1. BuLi
2. Me3SnCl
SnMe3
N
R
30, 91 %
31
Br Br
Pd(PPh3)4, CuO
m-CPBA
R
N
N
R
32, 30 %
R
N
N
R
O
O
33, 75 %

Figure 25

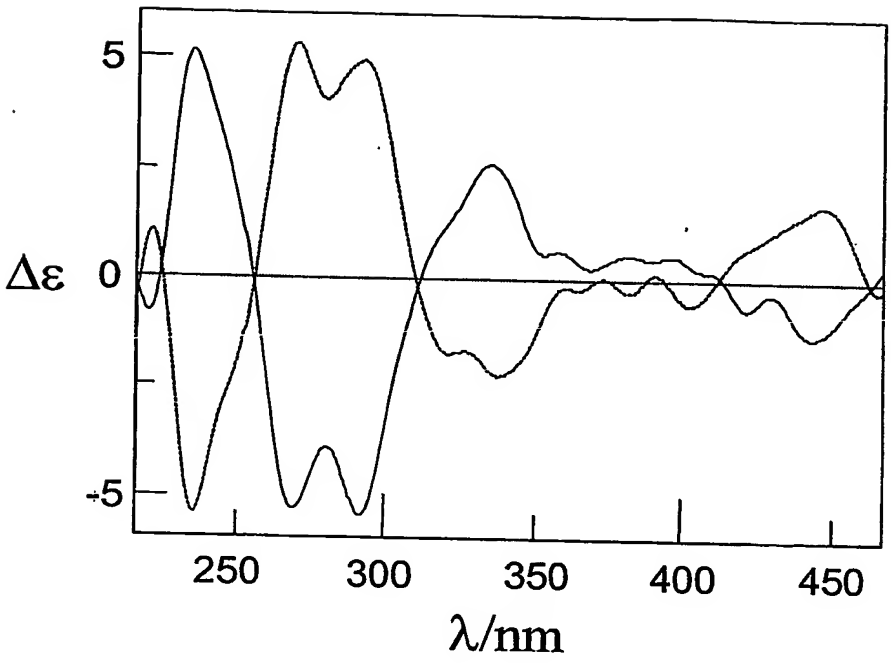
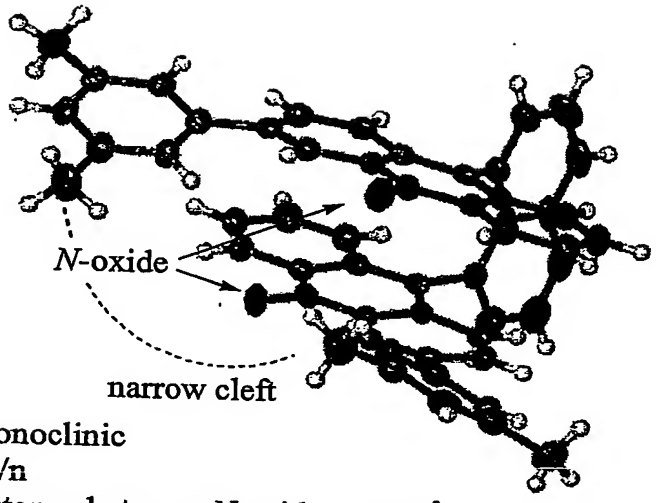


Figure 26



Monoclinic
P2/n
distance between *N*-oxides: 4.32 Å

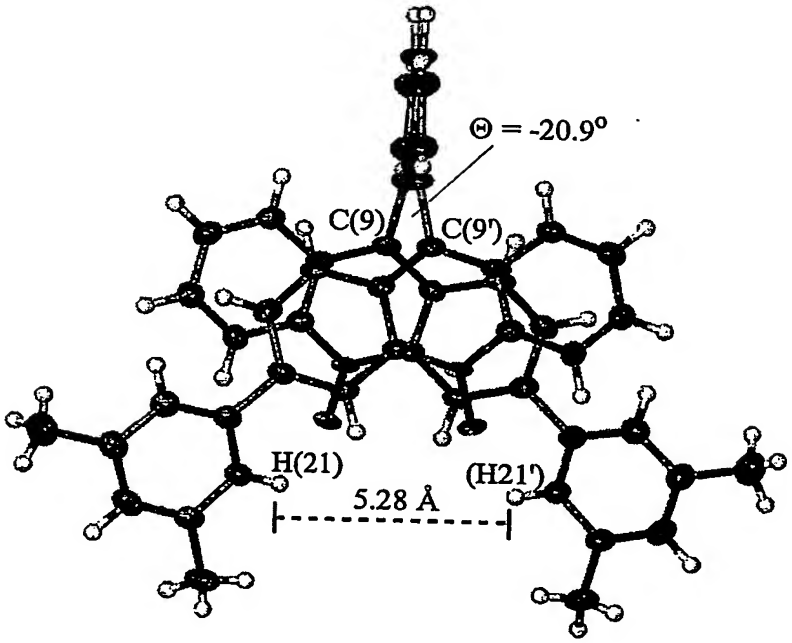
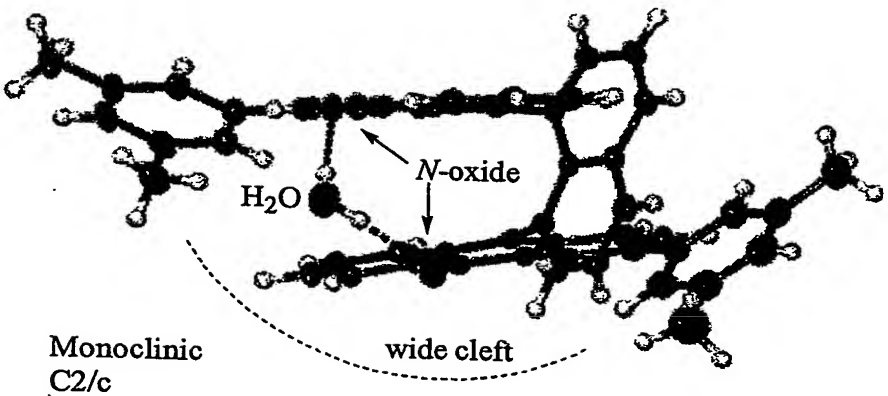


Figure 27



Monoclinic
C2/c
distance between *N*-oxides: 4.30 Å
hydrogen bond distance: 1.99 Å

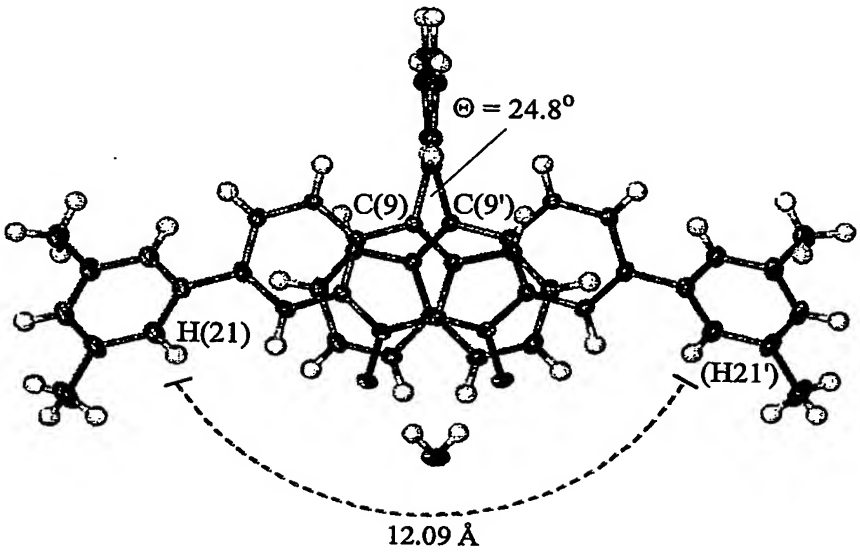


Figure 28

complex:	33-H_2O-CH_3CN	33-CH_2Cl_2
empirical formula	C28 H23 N2 O1.50	C27 H21 Cl2 N O
formula weight	411.48	446.35
temperature	186(2) K	183(2) K
wavelength	0.71073 Å	0.71073 Å
crystal system	Monoclinic	Monoclinic
space group	C2/c	P2/n
unit cell dimensions	a = 24.551(2) Å b = 13.3883(12) Å c = 13.7187(12) Å α= 90° β= 107.204(2)° γ = 90°	a = 13.839(2) Å b = 11.2871(18) Å c = 15.055(3) Å γ = 90° α= 90° β= 113.991(3)° γ = 90°
distance O-O	4.32 Å	4.30 Å
distance N-N	3.84 Å	3.82 Å
distance C(9)-C(9')	2.87 Å	2.91 Å
distance H(21)-H(21')	12.09 Å	5.28 Å
torsion Θ between acridyl rings	24.8°	-20.9°
Volume	4307.5(7) $Å^3$	2148.4(6) $Å^3$
Z	8	4
density (calculated)	1.269 Mg/m^3	1.380 Mg/m^3
Absorption coefficient	0.079 mm^{-1}	0.322 mm^{-1}
F(000)	1736	928
crystal size	0.95 x 0.46 x 0.46 mm^3	0.50 x 0.30 x 0.20 mm^3
theta range for data collection	1.74 to 27.00°.	1.69 to 25.00°.
index ranges	-31<=h<=31, -16<=k<=17, -17<=l<=17	-16<=h<=15, -13<=k<=10, -17<=l<=17
Reflections collected	18167	10895
independent reflections	4690 [R(int) = 0.0368]	3798 [R(int) = 0.0654]
completeness to theta = 27.00°	99.8 %	99.9 %
max. and min. transmission	0.9647 and 0.9289	0.9383 and 0.8554
refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
data / restraints / parameters	4690 / 0 / 292	3798 / 0 / 283
goodness-of-fit on F^2	1.090	0.875
final R indices [I>2sigma(I)]	R1 = 0.0568, wR2 = 0.1498	R1 = 0.0539, wR2 = 0.1284
largest diff. peak and hole	0.610 and -0.467 $e.Å^{-3}$	0.279 and -0.345 $e.Å^{-3}$

Figure 29

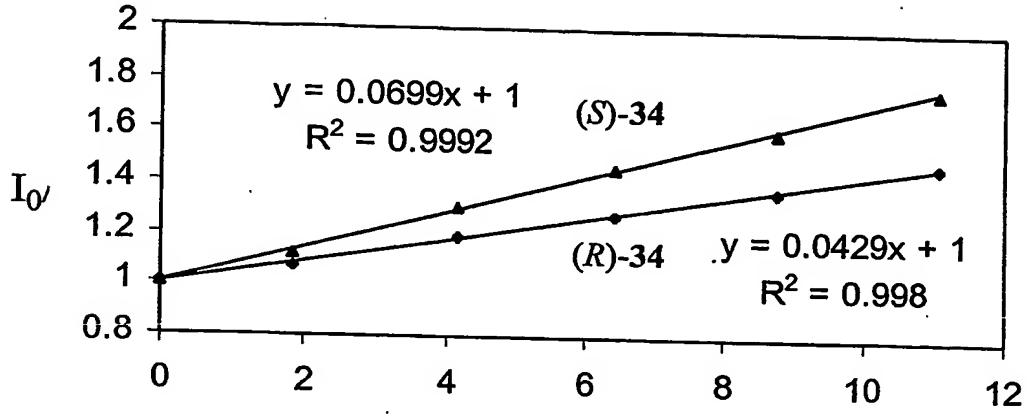

2
1.8
1.6
1.4
1.2
1
0.8
$I_0/$
y = 0.0699x + 1
R^2 = 0.9992
(S)-34
(R)-34
y = 0.0429x + 1
R^2 = 0.998
0
2
4
6
8
10
12

Figure 30

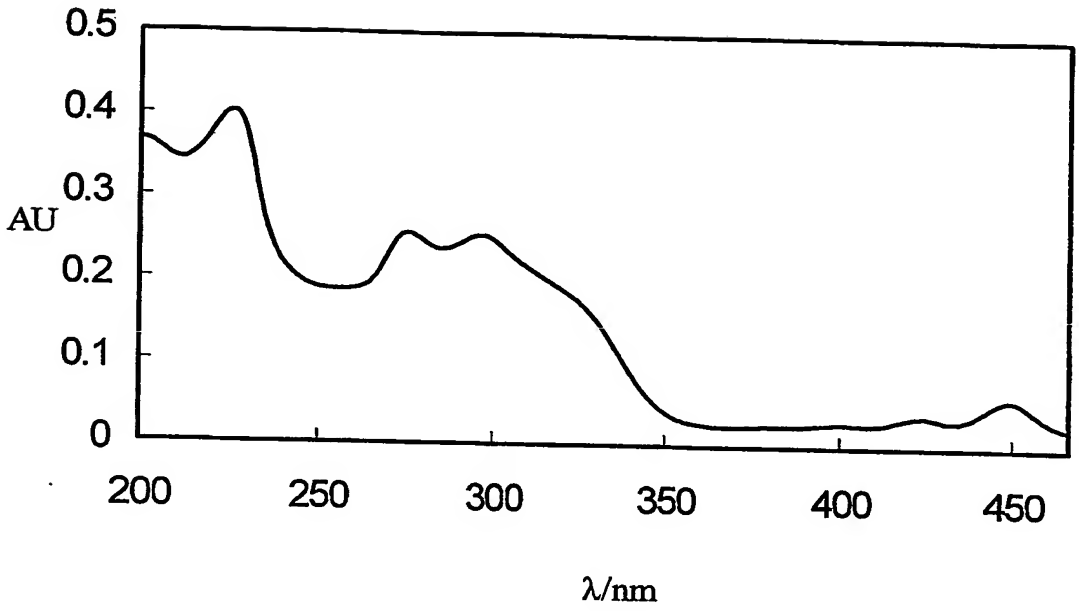


Figure 31

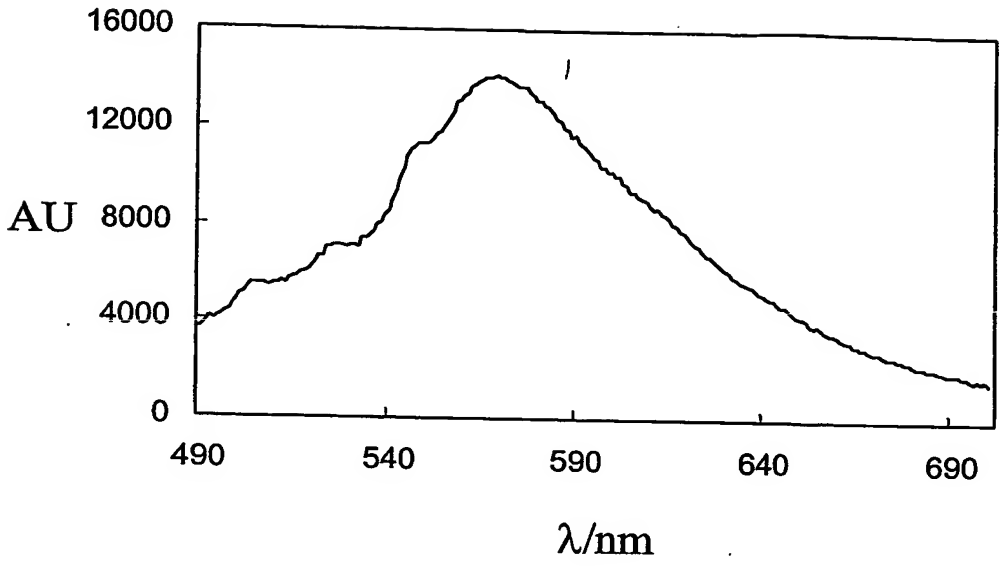


Figure 32

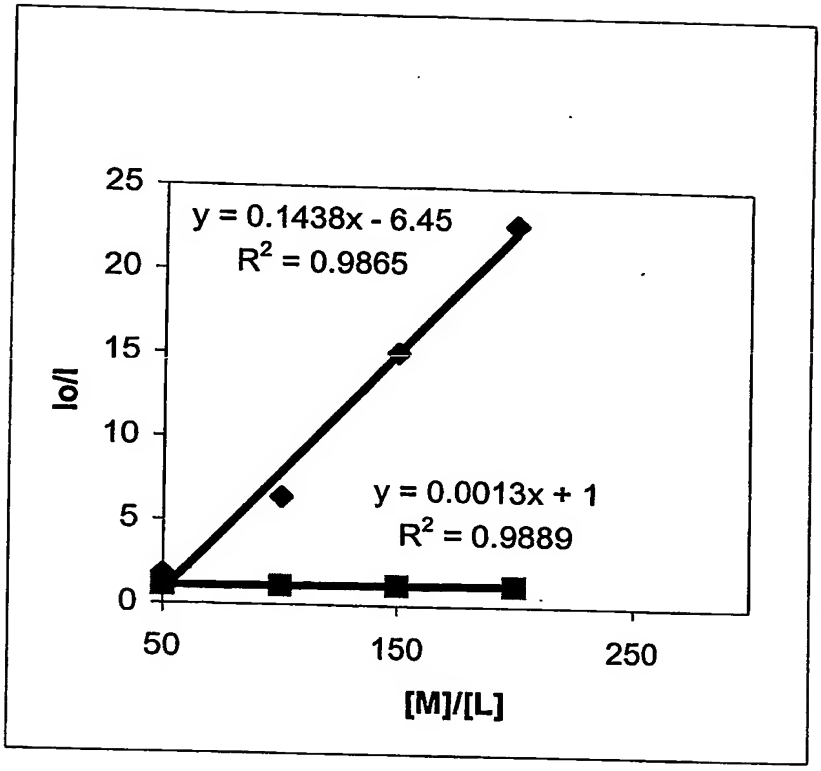

y = 0.1438x - 6.45
R2 = 0.9865
y = 0.0013x + 1
R2 = 0.9889
Io/I
[M]/[L]
0
5
10
15
20
25
50
150
250

Figure 33

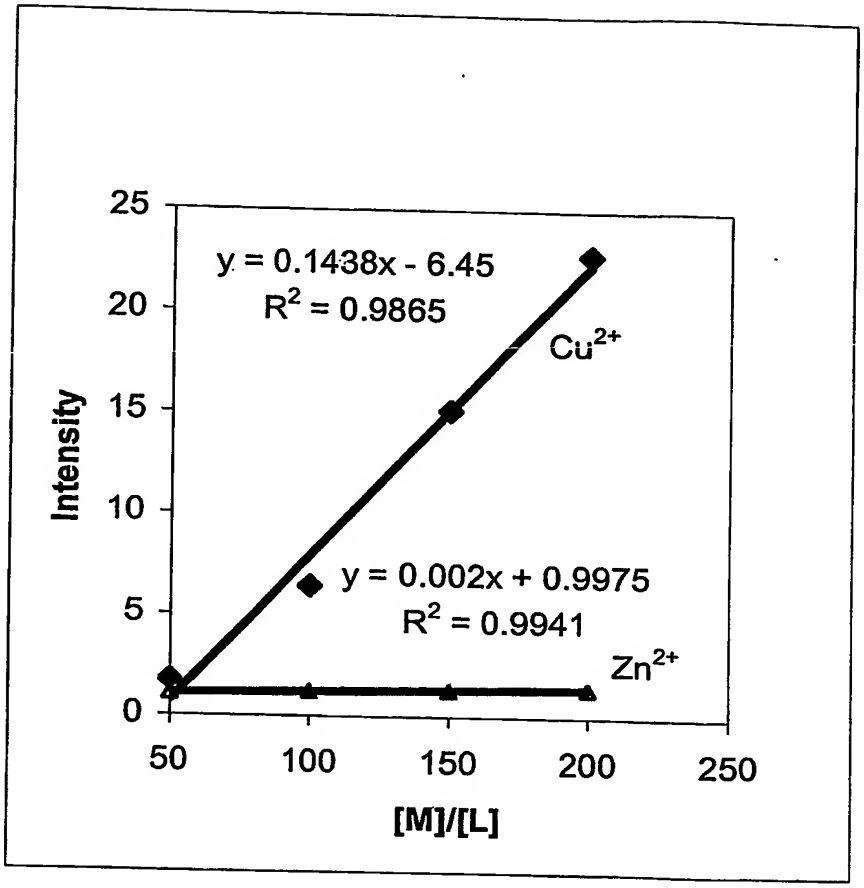

25
20
15
10
5
0
Intensity
y = 0.1438x - 6.45
R2 = 0.9865
Cu2+
y = 0.002x + 0.9975
R2 = 0.9941
Zn2+
50
100
150
200
250
[M]/[L]

Figure 34

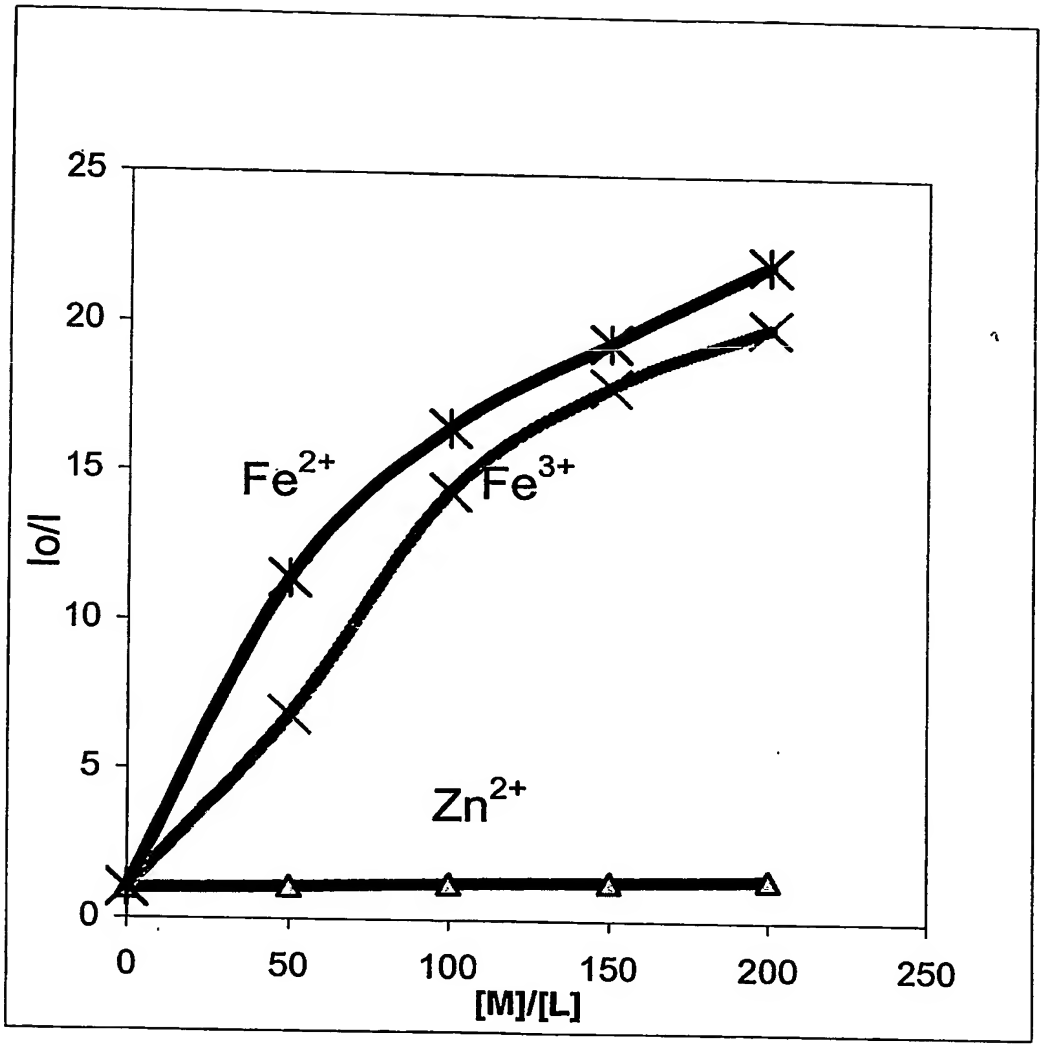


Figure 35

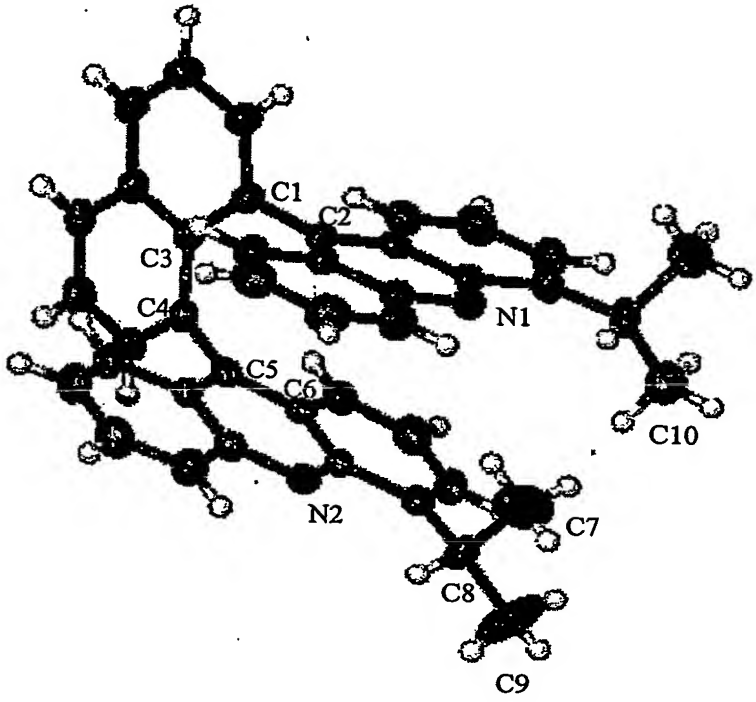


Figure 36

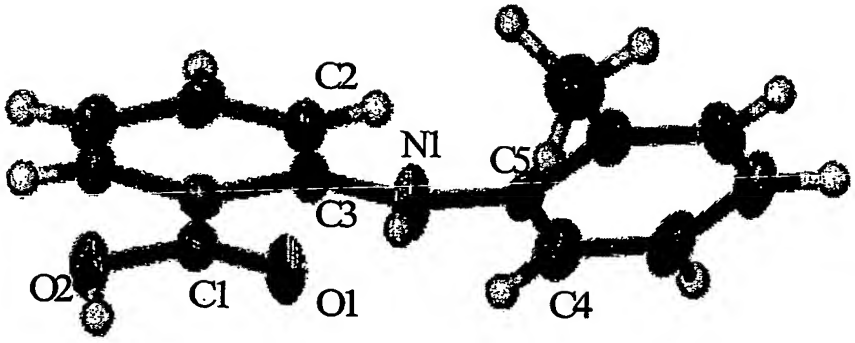


Figure 37

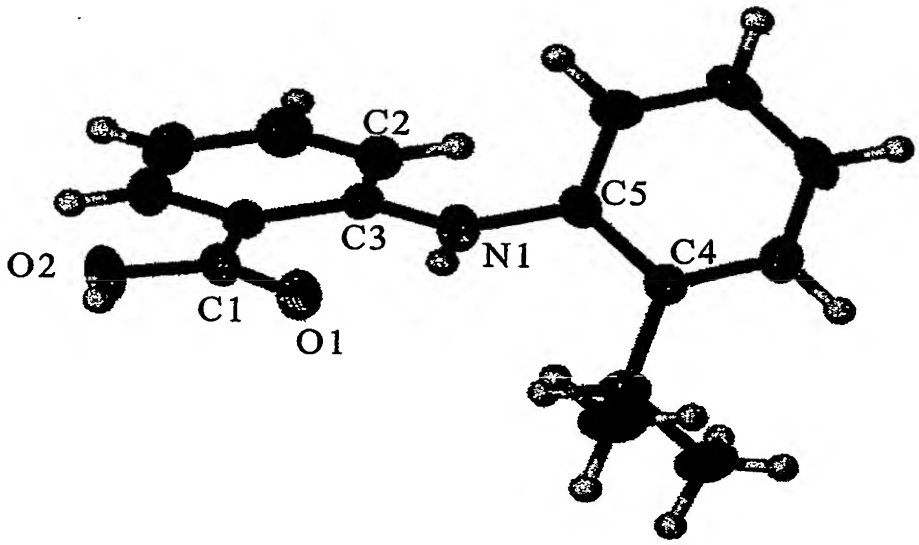


Figure 38

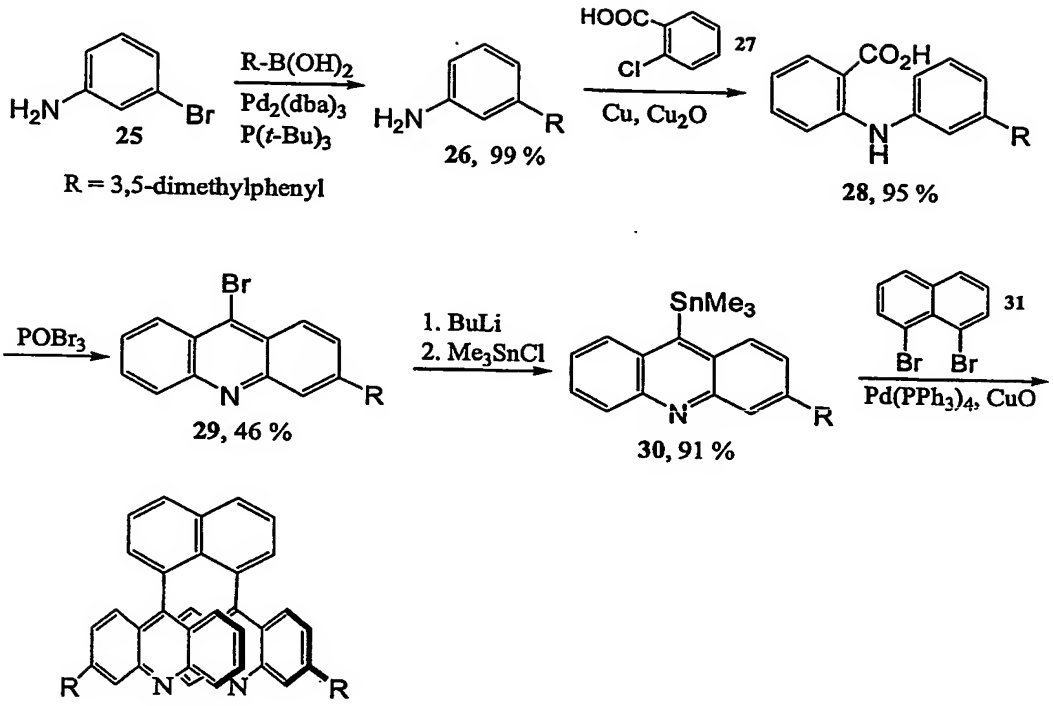

H2N
Br
25
R-B(OH)2
Pd2(dba)3
P(t-Bu)3
H2N
R
26, 99 %
HOOC
Cl
27
Cu, Cu2O
CO2H
N
H
R
28, 95 %
R = 3,5-dimethylphenyl
POBr3
Br
N
R
29, 46 %
1. BuLi
2. Me3SnCl
SnMe3
N
R
30, 91 %
31
Br Br
Pd(PPh3)4, CuO
R
N
N
R
32, 30 %

Figure 39

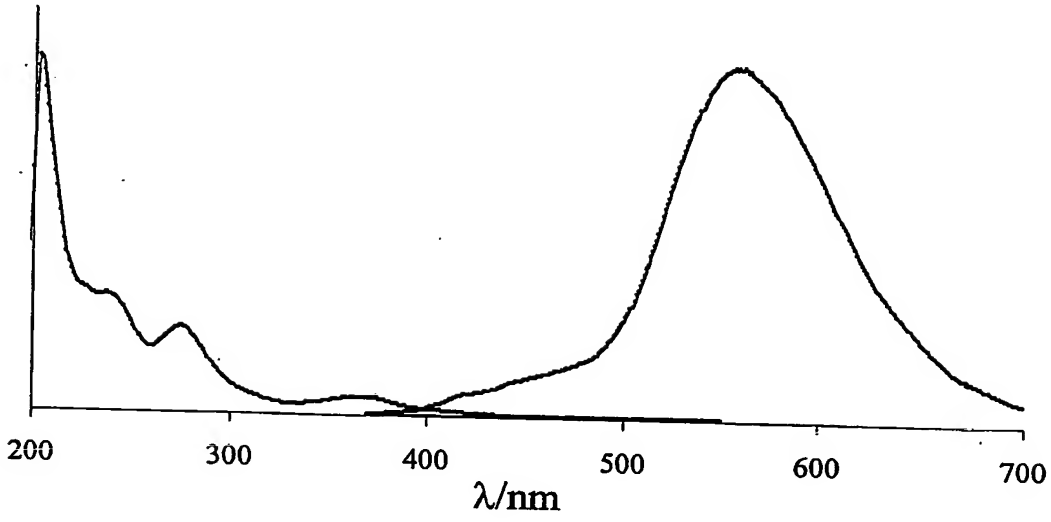


Figure 40

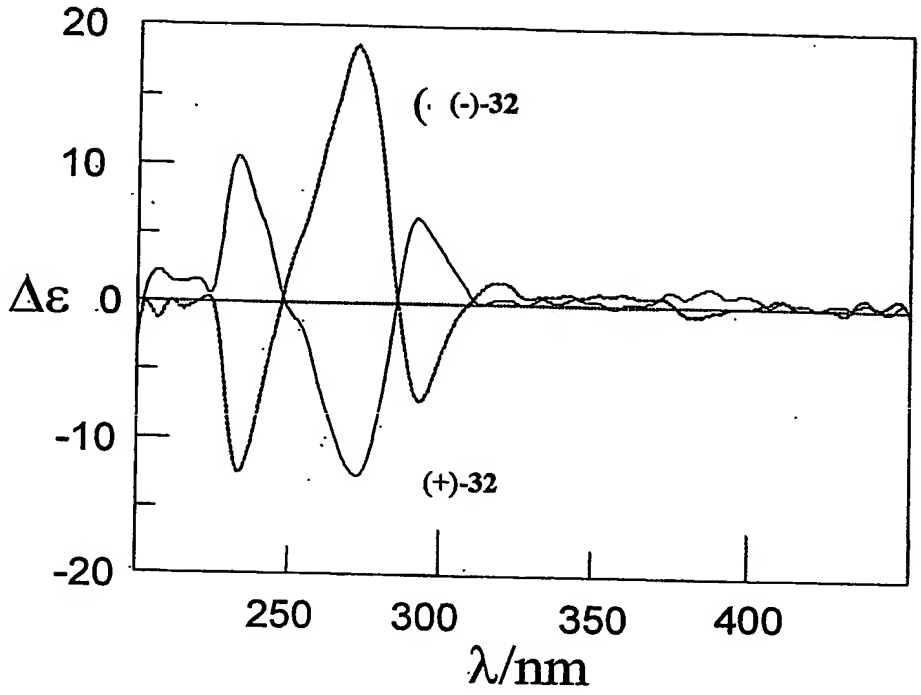


Figure 41

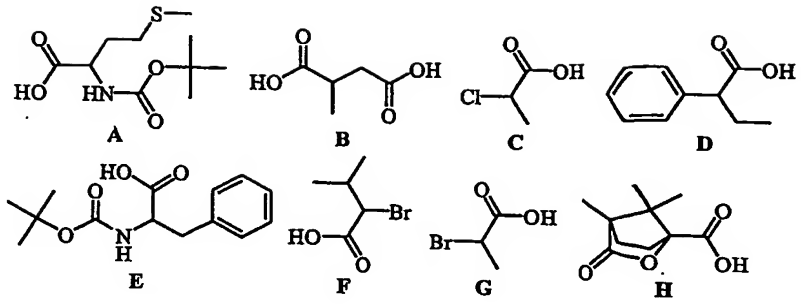


Figure 42

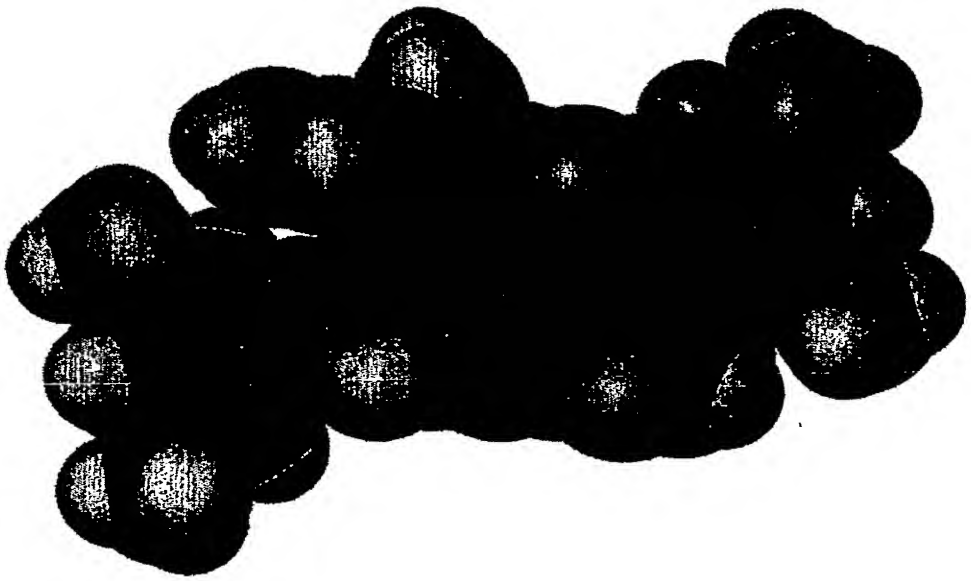


Figure 43

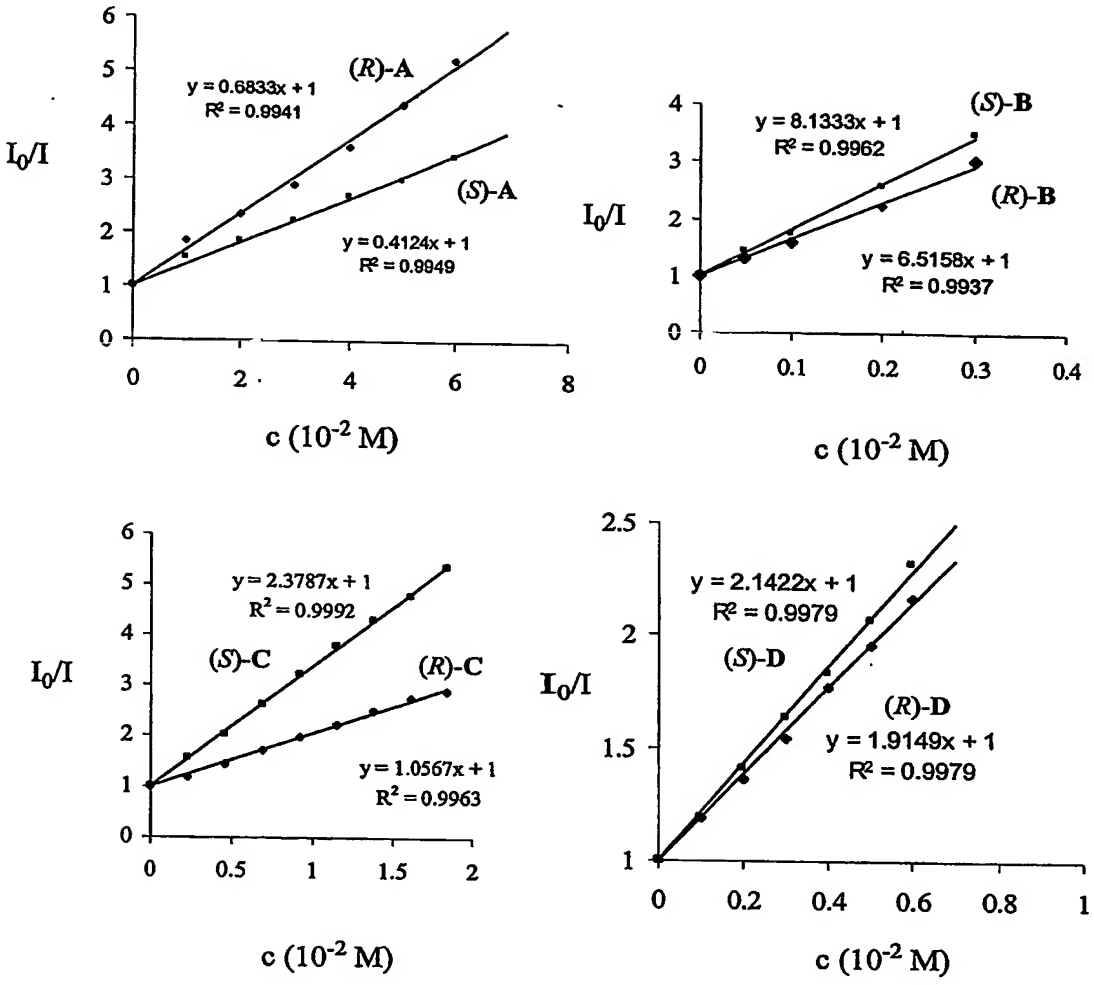

I0/I
y = 0.6833x + 1
R² = 0.9941
(R)-A
(S)-A
y = 0.4124x + 1
R² = 0.9949
c (10-2 M)
y = 8.1333x + 1
R² = 0.9962
(S)-B
(R)-B
y = 6.5158x + 1
R² = 0.9937
y = 2.3787x + 1
R² = 0.9992
(S)-C
(R)-C
y = 1.0567x + 1
R² = 0.9963
y = 2.1422x + 1
R² = 0.9979
(S)-D
(R)-D
y = 1.9149x + 1
R² = 0.9979

Figure 44

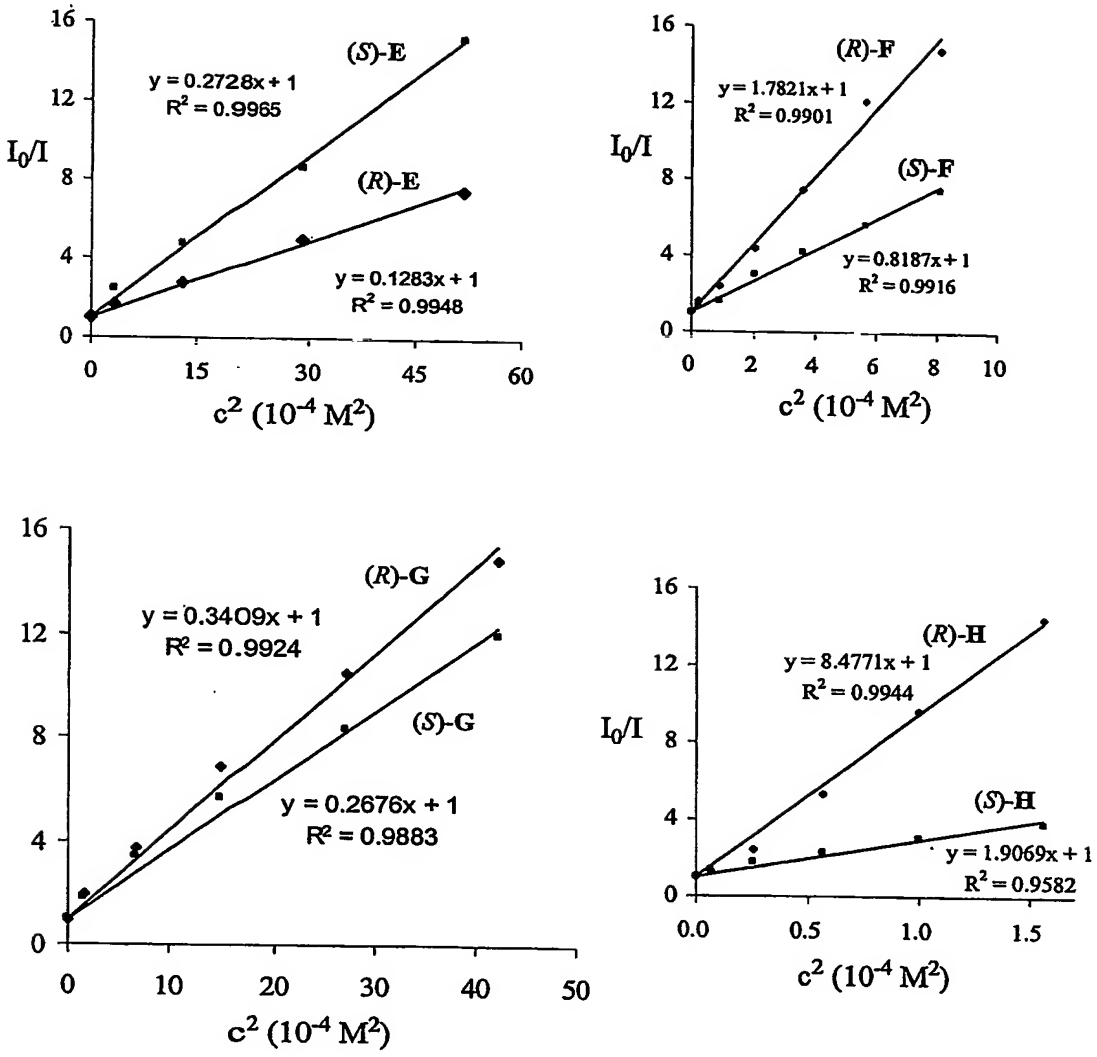

(S)-E
y = 0.2728x + 1
R² = 0.9965
(R)-E
y = 0.1283x + 1
R² = 0.9948
I0/I
c² (10⁻⁴ M²)
(R)-F
y = 1.7821x + 1
R² = 0.9901
(S)-F
y = 0.8187x + 1
R² = 0.9916
(R)-G
y = 0.3409x + 1
R² = 0.9924
(S)-G
y = 0.2676x + 1
R² = 0.9883
(R)-H
y = 8.4771x + 1
R² = 0.9944
(S)-H
y = 1.9069x + 1
R² = 0.9582

Figure 45

analyte	ratio (32/analyte)	α	$K_{(+)\text{-}1\text{-}(R)\text{-analyte}}$[a]	$K_{(+)\text{-}1\text{-}(S)\text{-analyte}}$[a]
A	1:1	1.7 (*R/S*)	88.5 M^{-1}	56.5 M^{-1}
B	1:1	1.3 (*S/R*)	610.0 M^{-1}	840.0 M^{-1}
C	1:1	2.2 (*S/R*)	75.6 M^{-1}	241.3 M^{-1}
D	1:1	1.1 (*S/R*)	18.4 M^{-1}	20.0 M^{-1}
E	1:2	2.1 (*S/R*)	2100.0 M^{-2}	4900.0 M^{-2}
F	1:2	2.2 (*R/S*)	16000.0 M^{-2}	7100.0 M^{-2}
G	1:2	1.3 (*R/S*)	5300.0 M^{-2}	4700.0 M^{-2}
H	1:2	4.5 (*R/S*)	63000.0 M^{-2}	36000.0 M^{-2}

[a]Obtained using the Benesi-Hildebrand equation for 1:1 complexes (**A-D**) and 1:2 complexes (**E-H**).

Figure 46

complex:	32	
Empirical formula	$C_{52} H_{38} N_2$	
Formula weight	690.84	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 16.1895(13) Å	α= 90°.
	b = 10.3998(9) Å	β= 92.680(2)°.
	c = 21.2941(18) Å	γ = 90°.
Volume	3581.3(5) $Å^3$	
Z	4	
Density (calculated)	1.281 mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	1456	
Crystal size	0.30 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.91 to 24.99°.	
Index ranges	-19<=h<=19, -12<=k<=12, -25<=l<=25	
Reflections collected	13111	
Independent reflections	3166 [R(int) = 0.0375]	
Completeness to theta = 24.99°	100.0 %	
Absorption correction	Multiscan	
Max. and min. transmission	0.9927 and 0.9782	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3166 / 0 / 247	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0485, wR2 = 0.1122	
R indices (all data)	R1 = 0.0697, wR2 = 0.1190	
Largest diff. peak and hole	0.182 and -0.147 $e.Å^{-3}$	

Figure 47

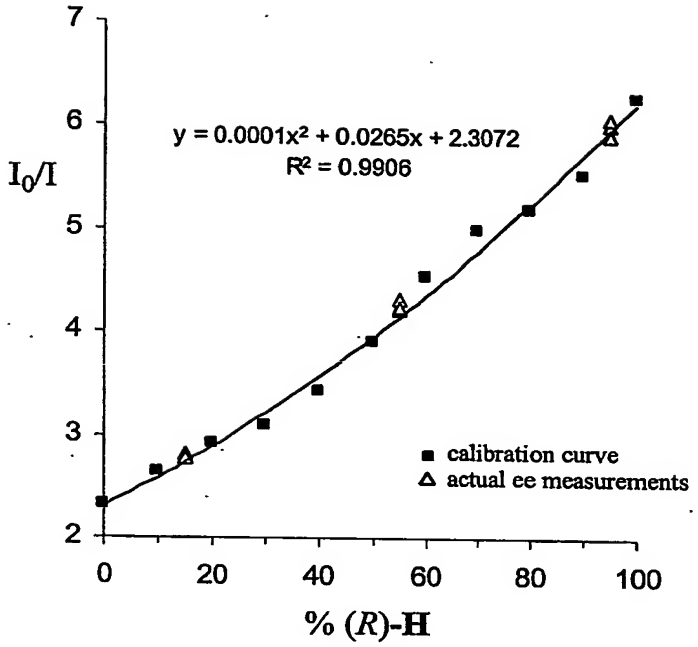

7
6
5
4
3
2
I_0/I
y = 0.0001x² + 0.0265x + 2.3072
R² = 0.9906
calibration curve
actual ee measurements
0
20
40
60
80
100
% (R)-H

Figure 48

% (*R*)	I	I_0/I
0	70354	2.324019
10	61948	2.639375
20	56011	2.919141
30	52849	3.093796
40	47734	3.425315
50	41878	3.904293
60	35989	4.543166
70	32725	4.996303
80	31520	5.18731
90	29509	5.540818
100	25983	6.29273

note: I_0 was 163504.

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